Numerical study of essentially unsteady evaporation

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Abstract. We study numerically essentially unsteady evaporation and heat transfer of a rarefied gas using the S-model kinetic equation. Three particular cases are considered: one-dimensional flow from a flat surface and purely radial flows from the surface of a cylinder or a sphere. We present numerical results for different values of the evaporation coefficient and saturated-vapor density which demonstrate the strong dependence of the flow on these two parameters.

INTRODUCTION

Physics of evaporation has been studied extensively in recent years. Reviews on the subject can be found in [1, 2]. The majority of studies deals with steady evaporation or assume that the flow develops a steady-state regime quickly, see e.g. [3, 4, 5, 6]. Moreover, in many cases the steady form of the kinetic equation is used to describe the process. However, there are two main objections to using a steady description of the process. Firstly, under certain conditions the steady solution may form very slowly or do not exist at all. Secondly, the boundary conditions at infinity for steady equations may be difficult to pose.

In the present work, which is an extension of [7, 8, 9], we study the unsteady problem of evaporation and heat transfer on the basis of the kinetic Boltzmann equation with the S-model collision integral [10, 11]. The unsteady formulation allows us to compute the steady solution properly, if it exists, and resolves the ambiguity in setting the boundary conditions at infinity. Three particular cases are considered: one-dimensional flow from a flat surface and purely radial flows from the surface of a cylinder or a sphere. The main aim of the study is to investigate the influence of the evaporation coefficient and saturated-vapor density on the flow pattern and the mass rate.

FORMULATION OF THE PROBLEM

To save space, we shall describe the problem only for the radial flow from the surface of a sphere. Other cases can be formulated in a similar way.

Consider the unsteady purely radial flow of a rarefied gas induced by evaporation and heat transfer from the surface of a sphere of radius a into the surrounding space containing vapor (gas) of the evaporating condensed matter. Initially the gas is at rest in equilibrium with the surface. The gas number density and temperature are n_∞, T_∞, respectively. At $t = 0$ the surface temperature rises to $T_w > T_\infty$ and remains constant for $t > 0$. This increase in temperature and corresponding values of saturated-vapor density and pressure initiates the mass and heat fluxes from the surface into the unperturbed gas resulting in a unsteady radial gas motion. The problem is formulated for the Boltzmann equation with the S-model collision operator [10, 11]. The velocity distribution function f depends on spatial coordinate in the radial direction r, time t, radial ξ_r and transversal $\xi_\perp$ components of molecular velocity. In the rest of the paper we shall use the non-dimensional form of the equation in which the following quantities serve as reference values of spatial coordinate r, time t, density n, velocity u, temperature T, viscosity μ, heat flux q and distribution function f:

$$a, \quad a/\sqrt{2RT_\infty}, \quad n_\infty, \quad \sqrt{2RT_\infty}, \quad T_\infty, \quad \frac{5}{16} m n_\infty \sqrt{2\pi RT_\infty}\lambda_\infty, \quad m n_\infty (2RT_\infty)^{3/2}, \quad n_\infty (2RT_\infty)^{-3/2}. \tag{1}$$

Here m is the molecule mass, λ_∞ is mean free path in the undisturbed gas. Let also ζ and ω be polar coordinates in ξ_r, $\xi_\perp$ variables: $\xi_r = \zeta\cos\omega$, $\xi_\perp = \zeta\sin\omega$. The S-model kinetic equation in variables r, ζ, ω reads as follows [11, 4]:

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$$\frac{\partial f}{\partial t}+\zeta\cos\omega\frac{\partial f}{\partial r}-\frac{\zeta\sin\omega}{r}\frac{\partial f}{\partial\omega}=\frac{1}{\tau}(f^{+}-f),\quad \frac{1}{\tau}=\frac{8}{5\sqrt{\pi}}\frac{nT}{\mu}\frac{1}{\mathrm{Kn}},\quad \mathrm{Kn}=\lambda_\infty/a,$$
$$f^{+}=f_M\left(1+\frac{4}{5}(1-\mathrm{Pr})S_r c_r(c^2-\frac{5}{2})\right),\quad f_M=n(\pi T)^{-3/2}\exp(-c^2), \tag{2}$$
$$c_r=(\zeta\cos\omega-u)/\sqrt{T},\quad S_r=2q/(nT^{3/2}),\quad c^2=((\zeta\cos\omega-u)^2+(\zeta\sin\omega)^2)/T.$$

Here $\mathrm{Kn}=\lambda_\infty/a$ is the Knudsen number. Note that in the non-dimensional form the surface of the sphere corresponds to $r=1$. Gas density, radial velocity, temperature and radial heat flux are defined as

$$n=2\pi\int_0^\infty\int_0^\pi\zeta^2 f\sin\omega d\omega d\zeta,\quad nu=2\pi\int_0^\infty\int_0^\pi\zeta^3 f\sin\omega\cos\omega d\omega d\zeta,\quad \frac{3}{2}nT+nu^2=2\pi\int_0^\infty\int_0^\pi\zeta^4 f\sin\omega d\omega d\zeta,$$
$$q=2\pi\int_0^\infty\int_0^\pi\frac{1}{2}(\zeta\cos\omega-u)\left[(\zeta\cos\omega-u)^2+(\zeta\sin\omega)^2\right]\zeta^2 f\sin\omega d\omega d\zeta. \tag{3}$$

Let us describe the initial and boundary conditions. At the initial time $t=0$ and at infinity the gas is at rest:

$$f(r,0,\zeta,\omega)=f(r\to\infty,t,\zeta,\omega)=\pi^{-3/2}\exp(-\zeta^2) \tag{4}$$

At the evaporating surface the boundary condition for $\xi_r=\zeta\cos\omega>0$ is formulated according to [12]. We assume that the molecules incident on the phase surface are divided into two groups: i) condensed molecules ii) molecules reflected from the surface in accordance with a diffusive law with total temperature accommodation. These groups correspond to molecular fluxes $\alpha\int_0^\infty\int_{\pi/2}^\pi 2\pi\zeta^3 f\sin\omega\cos\omega d\omega d\zeta$ and $(1-\alpha)\int_0^\infty\int_{\pi/2}^\pi 2\pi\zeta^3 f\sin\omega\cos\omega d\omega d\zeta$ respectively. Here α is the condensation coefficient and, at the same time, the evaporation coefficient. Therefore, for molecules moving from the phase interface we specify the following boundary condition:

$$f(1,t,\zeta,\omega)=[\alpha n_s+(1-\alpha)n_w](\pi T_w)^{-3/2}\exp(-\zeta^2/T_w) \tag{5}$$

Here n_s is the saturated vapor density at the surface temperature T_w whereas n_w corresponds to the reflected molecules and is determined by the impermeability condition for this group of molecules. In this case the factor $(1-\alpha)$ drops out and we have a standard expression

$$n_w=-\frac{4\pi^{3/2}}{\sqrt{T_w}}\int_0^\infty\int_{\pi/2}^\pi\zeta^3 f\cos\omega\sin\omega\, d\omega d\zeta$$

Finally, the mass rate through the evaporating surface is given by

$$M_{ev}=\alpha\left(\frac{n_s\sqrt{T_w}}{2\sqrt{\pi}}+\int_0^\infty\int_{\pi/2}^\pi\zeta^3 f\cos\omega\sin\omega\, d\omega d\zeta\right),\quad M_\infty=\frac{n_s\sqrt{T_w}-1}{2\sqrt{\pi}}. \tag{6}$$

Here M_∞ is the limiting value which corresponds to the pure free-molecular evaporation ($\alpha=1$, $\mathrm{Kn}=\infty$). We note that the expression for M_∞ is the same for all three cases (one-dimensional, cylindrical or spherical evaporation).

The formulated problem was solved numerically. The major difficulties are due to the presence of the thin Knudsen layer with large gradients of macroparameters, the large size of the computational domain containing unsteady moving fronts as well as smooth features and the need to ensure the conservation property of the numerical method with respect to the collision integral. To circumvent outlined difficulties we use an implicit TVD scheme [13] and the conservative procedure for calculation of macroparameters [14]. The chosen advection scheme allows us to resolve moving fronts on coarse spatial meshes and use large time steps in the Knudsen layer (typically Courant number up to 10^6). The conservative procedure of evaluating macroparameters maintains conservation property on coarse velocity meshes for arbitrarily small Knudsen numbers. We remark that this procedure can be viewed as an extension to the S-model equation a similar procedure developed in [6] for the simpler BGK model equation [15].

The overall numerical algorithm is written in a delta form, one-step and unsplit, that is advection and collision operators are treated simultaneously. Therefore it is well suited for computing the steady flow regimes if they exist.

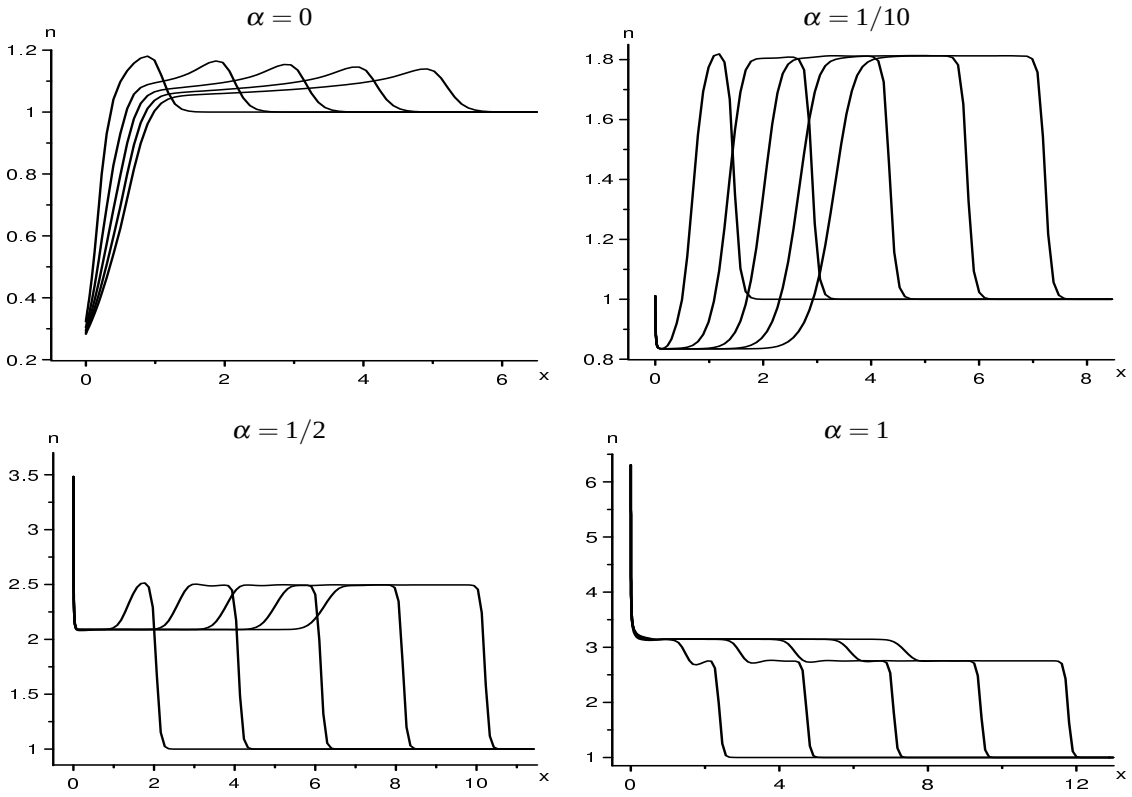

FIGURE 1. Density profiles for one-dimensional case. $T_w = 4$, $n_s = 10$, $\mathrm{Kn} = 10^{-2}$. Output times $t = 1, 2, 3, 4, 5$.

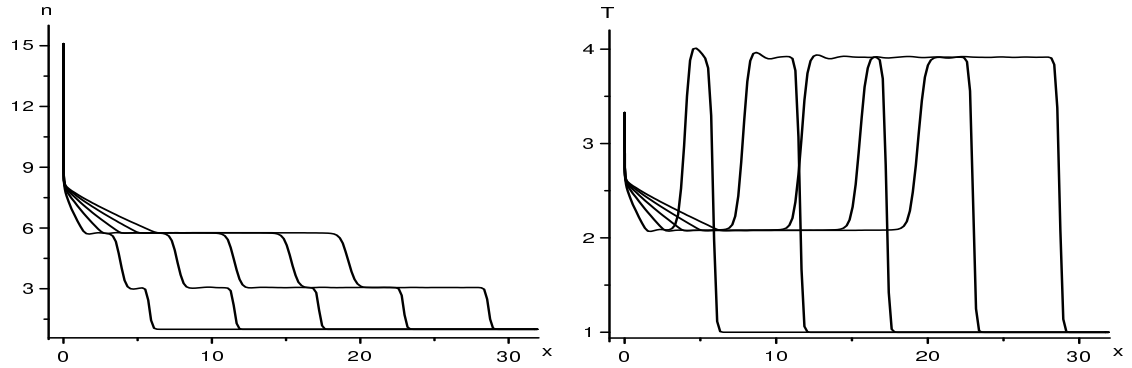

FIGURE 2. Density and temperature profiles for one-dimensional case. $T_w = 4$, $n_s = 25$, $\alpha = 1$, $\mathrm{Kn} = 10^{-2}$. Output times $t = 2, 4, 6, 8, 10$.

RESULTS

All results in the present work are obtained for the surface temperature $T_w = 4$, Knudsen number $\mathrm{Kn} = 10^{-2}$ and hard-sphere molecules ($\mu = \sqrt{T}$). For the given values of T_w and Kn we study the influence of the evaporation coefficient α and saturated-vapor density n_s on the flow. We remark that the case $\alpha = 1$ (no heat transfer) corresponds to the largest possible evaporation rate for a given surface temperature T_w whereas in the case $\alpha = 0$ there is no evaporation and only heat transfer takes place.

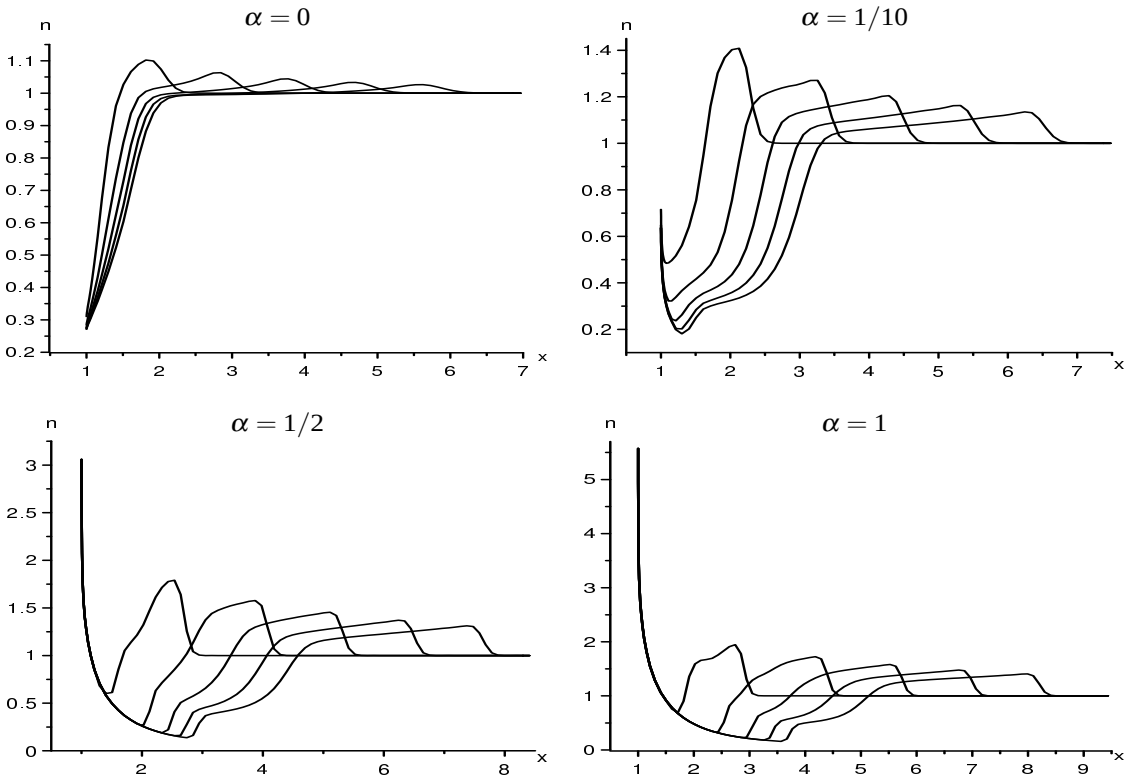

FIGURE 3. Density profiles for radial evaporation from a sphere. $T_w = 4$, $n_s = 10$, Kn $= 10^{-2}$. Output times $t = 1, 2, 3, 4, 5$.

Figure 1 illustrates density profiles for unsteady evaporation and heat transfer process in one space dimension for saturated-vapor density $n_s = 10$ and different values of evaporation coefficient $\alpha = 0$, $\frac{1}{10}$, $\frac{1}{2}$, 1. Since there is no characteristic length in the one-dimensional problem the Knudsen number here indicates the distance from which the flow is observed. We can see that the cases $\alpha = 0$ and $\alpha = 1$ differ qualitatively. At $\alpha = 1$ we have the standard pattern with a thin kinetic layer near evaporation surface, which becomes steady very rapidly with time. Outside it at a certain distance a uniform flow is formed which is connected by a thin mixing layer (contact discontinuity) with another uniform flow behind an outer shock wave propagating into the unperturbed gas. The contact discontinuity thus separates the newly-formed vapor and the gas compressed by the shock. Overall, the flow outside the Knudsen layer is similar to that induced by a piston moving with a constant velocity.

In the opposite limiting case $\alpha = 0$ a shock is again formed which speed and amplitude decrease with time. There are no uniform flow zones. Heat transfer from the surface occurs in a fairly thick layer in which the temperature decreases steeply while the density increases nearly linearly with the distance from the origin. The flow is thus unsteady for all times.

In the intermediate cases $\alpha = \frac{1}{10}$ and $\alpha = \frac{1}{2}$ the energy flux has both convective and molecular components. Qualitatively the behavior of the flow is determined by the presence of the convective part of the energy flux. The decrease of α as compared to the case $\alpha = 1$ leads to the natural decrease of the shock speed and to a certain redistribution of the flow parameters.

Figure 2 shows profiles of gas density and temperature for the case of a stronger pure evaporation corresponding to the saturated-vapor density $n_s = 25$ and condensation coefficient $\alpha = 1$. The qualitative difference from the moderate evaporation considered above is the appearance of an expanding (unsteady) zone *which does not coincide at all with the Knudsen layer* but has the same scale as the flow itself. In this zone the flow pattern is similar to that of the evaporation into vacuum [16]. Therefore, the flow near the phase interface cannot be described by the kinetic equation in the steady form. We also note that for $n_s = 25$ the uniform flow between the expanding unsteady zone and the contact discontnuity is actually *supersonic* with the Mach number $M \approx 1.45$.

TABLE 1. Normalized mass rate M_{ev}/M_∞ as a function of α for $n_s = 10$, $T_w = 4$, $\mathrm{Kn} = 10^{-2}$.

α	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
Flat surface	0.0	0.0954	0.1884	0.2791	0.3672	0.4524	0.5348	0.6142	0.6908	0.7645	0.8356
Cylinder	0.0	0.1030	0.2032	0.2989	0.3908	0.4792	0.5643	0.6460	0.7249	0.8011	0.8743
Sphere	0.0	0.1041	0.2050	0.3026	0.3969	0.4881	0.5764	0.6617	0.7444	0.8243	0.9018

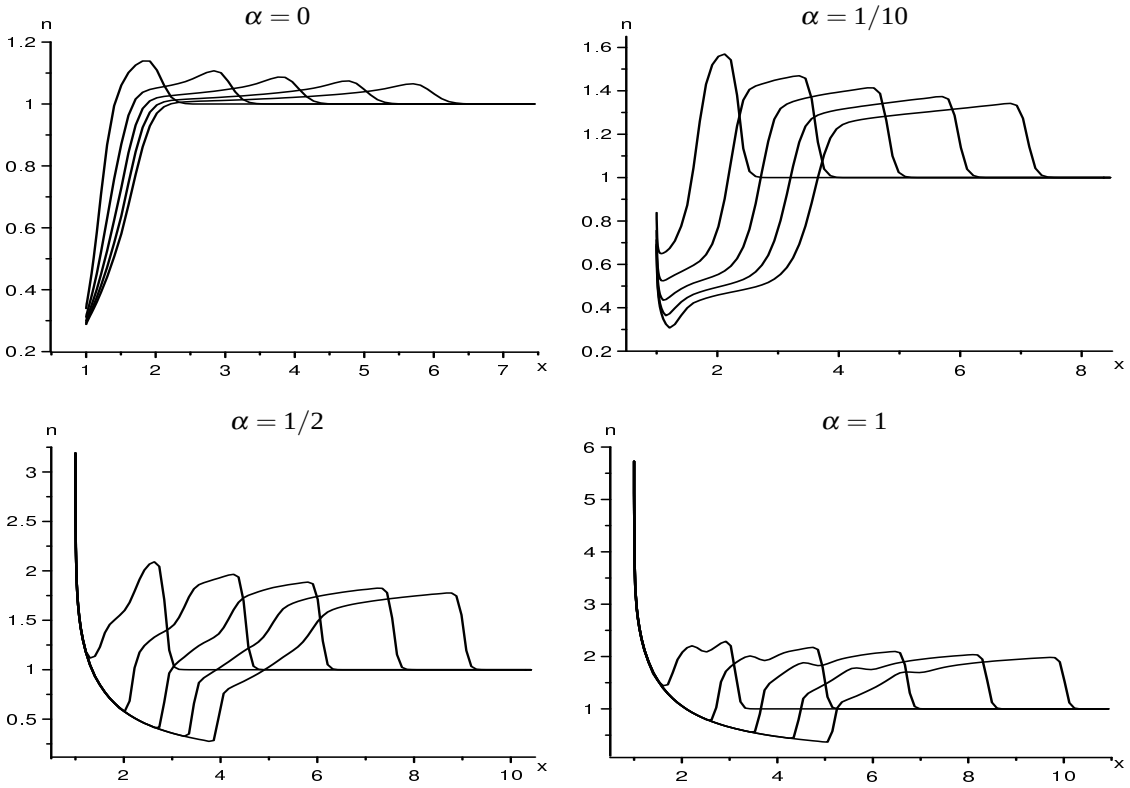

FIGURE 4. Density profiles for radial evaporation from a cylinder. $T_w = 4$, $n_s = 10$, $\mathrm{Kn} = 10^{-2}$. Output times $t = 1, 2, 3, 4, 5$.

Figure 3 illustrates the unsteady radial flow from the surface of a sphere for $n_s = 10$ and different values of evaporation coefficient $\alpha = 0$, $\frac{1}{10}$, $\frac{1}{2}$, 1. For the case of pure evaporation ($\alpha = 1$) the flow domain can be divided into an inner zone, which includes the Knudsen layer, and outer gasdynamic zone. In the inner zone the expansion of vapor results in a sharp decrease of gas density and temperature and increase in velocity. Qualitatively expansion develops according to a gasdynamic supersonic flow from a spherical source into vacuum and ends with an inner unsteady shock wave moving with a decreasing speed; as time evolves this shock wave becomes steady. It is important to realize that the inner shock wave connects *the supersonic and subsonic branches of the steady gasdynamical flow from a source*, see [17] for the detailed study in the steady radial evaporation from the sphere. On the other hand, in the outer zone the evaporated gas compresses the initially unperturbed vapor resulting in an outer shock wave. The two zones, inner and outer, are joined by a thin mixing layer which in the limiting case $\mathrm{Kn} \to 0$ becomes the contact discontinuity.

Overall, the structure of the fully developed flow in the case of pure evaporation ($\alpha = 1$) is as follows (from the surface of the sphere to infinity): supersonic flow from a source, the inner shock wave, subsonic flow from a source, the mixing layer (contact discontinuity) and the outer shock wave. As in the one-dimensional case, the contact discontinuity separates the newly-formed vapor and the gas compressed by the shock. In the steady formulation of the problem the boundary conditions at infinity correspond to the values of n, u and T between the inner shock wave and

the mixing layer [17].

In the opposite limiting case $\alpha = 0$ again a flow with a shock wave forms. The speed and amplitude of this shock are smaller than that for $\alpha = 1$. There are no stationary zones in the solution at any time. We note that for large times the external shock wave becomes a sound wave. Similar to the one-dimensional case, in the intermediate cases $\alpha = \frac{1}{10}$ and $\alpha = \frac{1}{2}$ the flow is qualitatively determined by the presence of the convective part of the energy flux. We note that when α is sufficiently small (e.g. $\alpha < \frac{1}{10}$) the inner shock wave merges with the Knudsen layer.

Figure 4 illustrates the unsteady radial flow from the surface of a cylinder for the saturated-vapor density $n_s = 10$ and different values of evaporation coefficient $\alpha = 0$, $\frac{1}{10}$, $\frac{1}{2}$, 1. Qualitatively the flow pattern is similar to that of Figure 3. However, there are significant differences in the scales of the flow and amplitudes of the waves, e.g. the outer shock wave for the cylindrical case vanishes slower and moves faster than that in the radial flow from the surface of a sphere.

We note that for the case of the pure evaporation ($\alpha = 1$) the behavior of the flow for large output times (up to $t = 50$) was studied in [8], [9] by solving the kinetic equation in the Knudsen layer near the evaporating surface and the Euler equations outside the kinetic layer.

Finally, Table 1 contains the normalized mass rate values M_{ev}/M_∞ as a function of the evaporation coefficient α for the saturated-vapor density $n_s = 10$. We observe that the dependence on α is weekly non-linear and that the closer the evaporating surface to the flat one the smaller the difference with the one-dimensional values of M_{ev}/M_∞ is.

CONCLUSIONS

We have studied numerically the unsteady evaporation and heat transfer of a rarefied gas for different values of the evaporation coefficient α and saturated-vapor density n_s. Three particular cases are considered: one-dimensional flow from a flat surface and radial flows from the surface of a cylinder or a sphere. The presented results illustrate a strong dependence of the flow on n_s and α. In particular, the steady-state regime near the evaporating surface may not exist for sufficiently small values of α or large values of n_s.

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